



## FYS3150/FYS4150: Computational Physics I

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# Project 5

## Variational Monte Carlo of Confined Electrons in a Pure Three-dimensional Isotropic Harmonic Oscillator Potential

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### Abstract

In this project, quantum mechanical expectation values for three-dimensional two-electron quantum dots, both with and without inter-electronic Coulomb interaction, were estimated using the variational Monte Carlo (VMC) method with the Metropolis algorithm. Two trial wave functions  $\Psi_{T_1}$  and  $\Psi_{T_2}$ , with the latter accounting for the electron-electron interaction and the former not, were constructed with optimal variational parameters found upon minimizing the total energy of the systems.

The simulated energy functional as a function of the variational parameter  $\alpha$  for the non-interacting system with  $\Psi_{T_1}$ , aligned very well with the corresponding closed-form expression. For the interacting system with  $\Psi_{T_2}$  and oscillator frequency  $\omega = 1$ , the upper bound estimate of the ground state energy was simulated, with  $N = 10^6$  Monte Carlo cycles, to be 3.730 a.u. (atomic units). Compared to the corresponding analytical value 3.558 a.u., it seems like the method struggles to yield a precise estimate of the energy in the interacting case. The virial theorem applied to a quantum harmonic oscillator,  $\langle T \rangle = \langle V \rangle$ , was tested for both the non-interacting and interacting system as a function of  $\omega$ . The former system corresponded well with the virial theorem, whereas the latter did not conform with the theorem. However, this was expected since the aforementioned virial relation is derived for a non-interacting quantum dot.

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# 1 Introduction

Most quantum mechanical problems involve systems with a large number of interacting electrons and ions or nucleons. As such, expectation values of quantum mechanical operators involve multidimensional integrals where an exact solution may be hard to find or not obtainable at all. The problem is that the exact wave function usually is unknown. Monte Carlo methods are ideal for such multidimensional integral problems, in particular the variational Monte Carlo (VMC) method which is based on the variational principle. The method is to construct trial wave functions that captures as much of the physical features of system as possible, with variational parameters that are optimized upon minimizing the total energy of the system.

In this project, the aim is to perform VMC computations with the Metropolis algorithm to evaluate the ground state energy, the mean relative distance between two electrons and expectation values of the kinetic and potential energies of quantum dots with  $N = 2$  electrons. The two electrons will be confined in a pure three-dimensional isotropic harmonic oscillator potential, both with and without Coulomb repulsion. Two trial wave functions  $\Psi_{T_1}$  and  $\Psi_{T_2}$ , with the latter accounting for the electron-electron interaction and the former not, will be used in order to evaluate the expectation values with the VMC method.

Analytical expressions for the local energy for  $\Psi_{T_1}$  and  $\Psi_{T_2}$ , i.e. for both the non-interacting and interacting system, will be derived, as this advantageous for the computation of the energy functional  $E[\Psi_T]$ . A closed-form expression for the energy functional in the non-interacting case will be derived as well, serving as a benchmark for the implementation of the numerical method. The quantum harmonic oscillator virial relation will also be formulated.

The implementation of the Metropolis algorithm in this project will be a so-called brute-force one, meaning that the algorithm will be manipulated into accepting roughly 50% of the proposed moves. This is accomplished by having the Metropolis random walker efficiently walk through configuration space with an imposed step length. An algorithm for optimizing the variational parameters will also be devised and implemented.

With the implementation in place, the expectation value of the energy and the energy variance as functions of the variational parameter  $\alpha$  will be studied for both the non-interacting and interacting system, with the aim to find the energy and variance minima as well as the optimal variational parameters.

Next, the stability of the calculations of the energy and energy variance as functions of the number of Monte Carlo cycles will be studied for different oscillator frequencies  $\omega$  and the interacting system with  $\Psi_{T_1}$ . These results will be compared with exact results provided by Taut [1] and results obtained with the Jacobi rotation method by the authors in [2]. Having found an optimal number of Monte Carlo cycles, the ground state energy, the mean relative distance between two electrons and expectation values of the kinetic and potential energies are computed for the interacting system with both  $\Psi_{T_1}$  and  $\Psi_{T_2}$ . The latter expectations values are then compared with the quantum harmonic oscillator virial relation.

This project is structured by first presenting a theoretical overview of the physical model, the aforementioned methods, and derivations of closed-form expressions in [Section 2](#). This is followed by a presentation on the approach to study the various computations of interest in [Section 3](#). Next, the results of the implementation are presented in [Section 4](#), before subsequently they and the approach are discussed and concluded upon in [Section 5](#) and

[Section 6](#), respectively. Lastly, an outline of possible continuations of the model, with respect to the implementation, are presented in [Section 7](#).

## 2 Theory

### 2.1 Pure Isotropic Harmonic Oscillator Potential

An idealized Hamiltonian for a system of  $N$  electrons confined in a pure three-dimensional isotropic harmonic oscillator, is given by [3]

$$H = \sum_i^N \left( -\frac{1}{2} \nabla_i^2 + \frac{1}{2} \omega^2 r_i^2 \right) + \sum_{i < j} \frac{1}{r_{ij}},$$

where  $\omega$  is the oscillator frequency, the  $r_i$ 's are the electron positions in the oscillator, and the  $r_{ij}$ 's are the inter-electronic distances. Here, natural units ( $\hbar = c = e = m_e = 1$ ) are used and energies are given in atomic units a.u. The electron distances  $r_i$  and  $r_{ij}$  are then dimensionless. The Hamiltonian consists of a standard non-interacting harmonic oscillator term,

$$H_0 = \sum_i^N \left( -\frac{1}{2} \nabla_i^2 + \frac{1}{2} \omega^2 r_i^2 \right),$$

and a term for the repulsive interaction between two electrons,

$$H_1 = \sum_{i < j} \frac{1}{r_{ij}},$$

with  $r_{ij} = \sqrt{\mathbf{r}_1 - \mathbf{r}_2}$ . In this project the number of electrons is limited to  $N = 2$ .

The wave function for two electrons in the ground state is defined as

$$\Phi(\mathbf{r}_1, \mathbf{r}_2) = C \exp\left(-\omega(r_1^2 + r_2^2)/2\right),$$

where  $C$  is a normalization constant. This wave function is invariant under the exchange of variables  $\Phi(\mathbf{r}_1, \mathbf{r}_2) = \Phi(\mathbf{r}_2, \mathbf{r}_1)$ , that is, the wave function is symmetric. The Pauli exclusion principle states that two identical fermions, such as electrons, cannot occupy the same quantum state simultaneously, meaning that the total wave function has to be antisymmetric. In order to adhere to the exclusion principle, the electrons must be in a singlet state where the spins are anti-aligned, which is antisymmetric with total spin  $S = 0$ .

### 2.2 Review of the Variational Method

For many important quantum mechanical problems it is not possible to factor the Hamiltonian in an exactly solvable part with a small perturbation. For these kind of problems, perturbation theory is not applicable and one has to turn to other methods. One of these methods is known as the variational method, which is based on proposing trial wave functions  $|\psi_T\rangle$ . Ideally,  $|\psi_T\rangle$  captures as much of physics of the system as possible. By introducing one or more parameters changing the shape of  $|\psi_T\rangle$ , the parameters can be varied in order to find an upper bound estimate of the ground state energy.

For an operator in Hilbert space the eigenfunctions form a complete set of states. Assuming that  $|\psi_n\rangle$  are the orthonormal eigenfunctions of the Hamiltonian  $H$ , such that  $H|\psi_n\rangle = E_n|\psi_n\rangle$ . The trial wave function may then be expanded in this basis [4, p. 332-333]

$$|\psi_T\rangle = \sum_n c_n |\psi_n\rangle$$

The normalization of this new state is given by

$$\langle\psi_T|\psi_T\rangle = \sum_{nm} c_m^* c_n \langle\psi_m|\psi_n\rangle = \sum_n |c_n|^2$$

The energy expectation value for this trial state is given by

$$\langle\psi_T|H|\psi_T\rangle = \sum_n |c_n|^2 E_n,$$

which means that the energy functional can be written as

$$E[\psi_T] = \frac{\langle\psi_T|H|\psi_T\rangle}{\langle\psi_T|\psi_T\rangle} \quad (2.1)$$

By picking out the lowest energy state, an upper bound on the true ground state energy is given by

$$E_0 \leq \frac{\langle\psi_T|H|\psi_T\rangle}{\langle\psi_T|\psi_T\rangle} \quad (2.2)$$

This can be rewritten on integral form by inserting a complete set of states, abbreviating  $\mathbf{r} = (\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$

$$\mathcal{J} = \int d\mathbf{r} |\mathbf{r}\rangle \langle\mathbf{r}|$$

then the energy functional is equal to

$$E[\Psi_T] = \frac{\int d\mathbf{r} \Psi_T^*(\mathbf{r}) H \Psi_T(\mathbf{r})}{\int d\mathbf{r} \Psi_T^*(\mathbf{r}) \Psi_T(\mathbf{r})} \quad (2.3)$$

To summarize, the variational method in the form of an algorithm is [5, p. 461]

1. Construct a trial many-particle wave function  $\Psi_T(\mathbf{r}; \boldsymbol{\alpha})$  for  $N$  particles located at positions  $\mathbf{r} = (\mathbf{r}_1, \dots, \mathbf{r}_N)$ , depending on  $m$  variational parameters  $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_m)$ .
2. Evaluate the expectation value of the energy using [Equation \(2.3\)](#)
3. Vary the parameters  $\boldsymbol{\alpha}$  according to some minimization algorithm and return to the first step.

The above loop stops when the minimum of the energy according to some specified criterion is reached.

## 2.3 Variational Monte Carlo Sampling

Following the procedure presented by Lester & Hammond [6, p. 49-52], the energy functional can be rewritten by defining the local energy

$$E_L = \frac{1}{\Psi_T} H \Psi_T \quad (2.4)$$

Equation (2.3) then assumes the form

$$E[\Psi_T] = \frac{\int d\mathbf{r} |\Psi_T|^2 E_L(\mathbf{r})}{\int d\mathbf{r} |\Psi_T|^2} \equiv \int d\mathbf{r} P(\mathbf{r}) E_L(\mathbf{r}) = \langle E_L \rangle_{\Psi_T^2} \quad (2.5)$$

With this definition the energy functional has been expressed as a weighted average, instead of working with operator expectation values. The average is taken with respect to the distribution  $|\Psi_T|^2$ , and the normalized probability density function is

$$P(\mathbf{r}) = \frac{|\Psi_T|^2}{\int d\mathbf{r} |\Psi_T|^2} \quad (2.6)$$

Another useful property of the definition provided by Equation (2.4), is that the local energy is constant, meaning that the variance is zero, when  $\Psi_T$  is an eigenfunction of  $H$ . This is almost never the case, but the more accurate  $\Psi_T$  is, the smaller the variance in  $E_L$  will be.

In general the probability distribution Equation (2.6) is hard to calculate for multiple particles, especially the normalization factor in the denominator. The distribution is also likely close to zero for most of configuration space, making it very inefficient to the integration Equation (2.5) over a uniform area. In these circumstances the Metropolis algorithm is a good method to sample from  $|\Psi|^2$ . The algorithm will be laid out in detail in the next section.

By letting  $\{X\}$  denote the sampled points, the estimate of the energy is given by

$$E[\Psi_T] = \langle E_L \rangle_{\Psi_T^2} = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^N E_L(X_i) \quad (2.7)$$

and the variance

$$\sigma^2(E[\Psi_T]) = \langle E_L^2 \rangle_{\Psi_T^2} - \langle E_L \rangle_{\Psi_T^2}^2 \quad (2.8)$$

## 2.4 The Metropolis Algorithm

The Metropolis algorithm is a Markov chain Monte Carlo (MCMC) method for sampling the expectation of a statistic. A Markov chain is used to model the evolution of the system by generating a sequence of consecutive states, where each new state depend solely on the previous state. The Markov chain must adhere to the ergodic principle, that is, the system must have a non-zero probability of being able to assume all possible states during the process. Samples of a statistic are collected by performing  $N$  experiments in a so-called Monte Carlo simulation. One such experiment constitutes a Monte Carlo cycle. A statistic occurring  $M$  times thus have the probability  $M/N$  [5, p. 381-382].

For any choice of trial wave function, the local energy and probability distribution are given by Equation (2.4) and Equation (2.6). As previously stated, the probability distribution given by  $P(\mathbf{r})$  is hard to evaluate directly for a large number of particles. Thus, a Metropolis approach is preferred as it relies on ratios of probabilities, rather than the probabilities themselves. For the system of two electrons in a harmonic oscillator, the initial state can be described by a set of coordinates  $\mathbf{r}_i$  for the position of the electrons. To generate the next state  $\mathbf{r}_{i+1}$ , the procedure is to propose moving the electrons a small random step in some direction, one at a time. The chance of accepting the move is given by the acceptance amplitude, that is, the ratio of the probabilities of the new and the old state

$$A = \frac{\frac{|\Psi_{i+1}|^2}{\int d\mathbf{r} |\Psi|^2}}{\frac{|\Psi_i|^2}{\int d\mathbf{r} |\Psi|^2}} = \frac{|\Psi_{i+1}|^2}{|\Psi_i|^2} \quad (2.9)$$

Note how the troublesome normalizing factors cancel, so there is no need to calculate them. If the proposed state is more probable than the previous, that is  $A > 1$ , the state is always accepted. Otherwise, the new state is accepted if  $r < A$ , where  $r$  is a random number uniformly distributed on  $[0, 1]$ .

## 2.5 Closed-form Expressions for the Local Energy

As defined in Section 2.3, the local energy is found by evaluating

$$E_L = \frac{1}{\Psi} H \Psi$$

By using the trial wave function

$$\Psi_{T_1}(\mathbf{r}_1, \mathbf{r}_2) = C \exp(-\alpha\omega^2(r_1^2 + r_2^2)/2) \quad (2.10)$$

and the non-interacting Hamiltonian

$$H_0 = \sum_{i=1}^N \left( -\frac{1}{2} \nabla_i^2 + \frac{1}{2} \omega r_i^2 \right),$$

where the radial part of the differential operator is

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right),$$

the action of the two electron Hamiltonian on this trial wave function is

$$H_0 \Psi_{T_1} = -\frac{1}{2} (\nabla_1^2 \Psi_{T_1} + \nabla_2^2 \Psi_{T_1}) + \frac{1}{2} \omega^2 (r_1^2 + r_2^2) \Psi_{T_1}$$

For simplicity, the terms can be evaluated separately. The first term evaluates to

$$\begin{aligned} \nabla_1^2 \Psi_{T_1} &= \frac{1}{r_1^2} \frac{\partial}{\partial r} \left( -\alpha\omega r_1^3 \Psi_{T_1} \right) \\ &= -3\alpha\omega \Psi_{T_1} + (\alpha\omega r_1)^2 \Psi_{T_1} \end{aligned}$$

The same holds for the second term. Collecting all terms yields

$$\begin{aligned} H_0 \Psi_{T_1} &= \left[ -\frac{1}{2} \left( -6\alpha\omega + \alpha^2\omega^2(r_1^2 + r_2^2) \right) + \frac{1}{2}\omega^2(r_1^2 + r_2^2) \right] \Psi_{T_1} \\ &= \left[ 3\alpha\omega - \frac{1}{2}\alpha^2\omega^2(r_1^2 + r_2^2) + \frac{1}{2}\omega^2(r_1^2 + r_2^2) \right] \Psi_{T_1} \\ &= \left[ 3\alpha\omega + \frac{1}{2}\omega^2(r_1^2 + r_2^2)(1 - \alpha^2) \right] \Psi_{T_1} \end{aligned}$$

By the definition of the local energy, the wave functions will cancel and result in

$$E_{L_1}^0 = \frac{1}{2}\omega^2(r_1^2 + r_2^2)(1 - \alpha^2) + 3\alpha\omega \quad (2.11)$$

By including the interacting term, the local energy is just

$$E_{L_1}^1 = \frac{1}{2}\omega^2(r_1^2 + r_2^2)(1 - \alpha^2) + 3\alpha\omega + \frac{1}{r_{12}} \quad (2.12)$$

The second trial wave function is defined as

$$\Psi_{T_2}(\mathbf{r}_1, \mathbf{r}_2) = C \exp \left( -\alpha\omega^2 (r_1^2 + r_2^2) / 2 \right) \exp \left( \frac{r_{12}}{2(1 + \beta r_{12})} \right) \quad (2.13)$$

By applying the interacting Hamiltonian on this trial wave function, it can, in a similar fashion as above, be shown that the local energy is given by

$$E_{L_2}^1 = E_{L_1}^1 + \frac{1}{2(1 + \beta r_{12})^2} \left\{ \alpha\omega r_{12} - \frac{1}{2(1 + \beta r_{12})^2} - \frac{2}{r_{12}} + \frac{2\beta}{1 + \beta r_{12}} \right\} \quad (2.14)$$

The first trial wave function satisfies the cusp condition when  $r_{12} \rightarrow 0$  with the non-interacting Hamiltonian, but with the interacting Hamiltonian it does not. The second trial wave function on the other hand satisfies the cusp condition for the interacting case, due to the additional Jastrow factor.

## 2.6 Closed-form Expression for the Energy Functional

By considering the non-interacting system and using the trial wave function given by [Equation \(2.10\)](#), the analytical expression for the energy functional in [Equation \(2.1\)](#) can be found. The point of departure is

$$E[\Psi_{T_1}] = \frac{\int d\mathbf{r} |\Psi_{T_1}|^2 E_L(\mathbf{r})}{\int d\mathbf{r} |\Psi_{T_1}|^2} = \frac{I}{I_N},$$

with

$$|\Psi_{T_1}|^2 = |C|^2 \exp \left( -\alpha\omega (r_1^2 + r_2^2) \right)$$

In order to simplify the calculation of the integrals, it is advantageous to evaluate them in spherical coordinates

$$x = r \cos \theta \sin \phi, \quad y = r \sin \theta \sin \phi, \quad z = r \cos \phi,$$



with Jacobian  $J = r^2 \sin \theta dr d\theta d\phi$ . The normalization integral is then

$$I_N = |C|^2 \int dr_1 d\theta_1 d\phi_1 r_1^2 \sin \theta_1 \exp(-\alpha\omega r_1^2) \int dr_2 d\theta_2 d\phi_2 r_2^2 \sin \theta_2 \exp(-\alpha\omega r_2^2)$$

Each angular integral gives a factor of  $4\pi$ , and the remaining integrals are Gaussian integrals

$$\begin{aligned} I_N &= 16\pi^2 |C|^2 \int dr_1 r_1^2 \exp(-\alpha\omega r_1^2) \int dr_2 r_2^2 \exp(-\alpha\omega r_2^2) \\ &= 16\pi^2 |C|^2 \left( \frac{1}{2\alpha\omega} \sqrt{\frac{\pi}{\alpha\omega}} \right) \left( \frac{1}{2\alpha\omega} \sqrt{\frac{\pi}{\alpha\omega}} \right) \\ &= 16\pi^2 |C|^2 \left( \frac{\pi}{4(\alpha\omega)^3} \right) \end{aligned}$$

The integral in the numerator has the same angular dependence, so it will give the same factor  $16\pi^2$  as above. Writing out the local energy, the integral becomes

$$\begin{aligned} I &= 16\pi^2 |C|^2 \left[ \int dr_1 dr_2 r_1^2 r_2^2 \exp(-\alpha\omega(r_1^2 + r_2^2)) \left( \frac{\omega^2}{2} (1 - \alpha^2) (r_1^2 + r_2^2) + 3\alpha\omega \right) \right] \\ &= 16\pi^2 |C|^2 [I_1 + I_2], \end{aligned}$$

where

$$\begin{aligned} I_1 &= \frac{\omega^2}{2} (1 - \alpha^2) \left[ \int dr_1 r_1^4 \exp(-\alpha\omega r_1^2) \int dr_2 r_2^2 \exp(-\alpha\omega r_2^2) \right. \\ &\quad \left. + \int dr_1 r_1^2 \exp(-\alpha\omega r_1^2) \int dr_2 r_2^4 \exp(-\alpha\omega r_2^2) \right] \\ &= \frac{\omega^2}{2} (1 - \alpha^2) \left[ \left( \frac{3}{4(\alpha\omega)^2} \sqrt{\frac{\pi}{\alpha\omega}} \right) \left( \frac{1}{2\alpha\omega} \sqrt{\frac{\pi}{\alpha\omega}} \right) + \left( \frac{3}{4(\alpha\omega)^2} \sqrt{\frac{\pi}{\alpha\omega}} \right) \left( \frac{1}{2\alpha\omega} \sqrt{\frac{\pi}{\alpha\omega}} \right) \right] \\ &= \left( \frac{\pi}{4(\alpha\omega)^3} \right) \left[ \frac{3\omega}{2\alpha} (1 - \alpha^2) \right] \end{aligned}$$

and

$$I_2 = 3\alpha\omega \int dr_1 r_1^2 \exp(-\alpha\omega r_1^2) \int dr_2 r_2^2 \exp(-\alpha\omega r_2^2) = 3\alpha\omega \left( \frac{\pi}{4(\alpha\omega)^3} \right)$$

Collecting all terms gives

$$E[\Psi_{T_1}] = \frac{16\pi^2 |C|^2 \left( \frac{\pi}{4(\alpha\omega)^3} \right) \left( \frac{3\omega}{2\alpha} (1 - \alpha^2) + 3\alpha\omega \right)}{16\pi^2 |C|^2 \left( \frac{\pi}{4(\alpha\omega)^3} \right)}$$

Thus, the closed-form expression for the energy is

$$E[\Psi_{T_1}] = \frac{3\omega}{2\alpha} (1 - \alpha^2) + 3\alpha\omega \quad (2.15)$$

## 2.7 The Virial Theorem

In 1870, Rudolf Clausius gave several lectures [7] where he presented the idea known today as the virial theorem. The theorem states that for a bound system of  $N$  particles, the time average over the kinetic energy is related to the total potential energy by

$$\langle T \rangle = -\frac{1}{2} \sum_{i=1}^N \langle \mathbf{F}_i \cdot \mathbf{r}_i \rangle$$

where  $\mathbf{F}_i$  denotes the force acting on the  $i$ th particle at position  $\mathbf{r}_i$ . This theorem was originally expressed in classical mechanics, but is also applicable in quantum mechanics. The quantum analogy can be found by using Ehrenfest's theorem [4, p. 86], which relates the time derivative of a time averaged operator to the time averaged commutator of that operator with the Hamiltonian

$$\frac{d}{dt} \langle A \rangle = i \langle [H, A] \rangle + \left\langle \frac{\partial A}{\partial t} \right\rangle$$

By defining the explicitly time independent operator,  $A = \mathbf{r} \cdot \mathbf{p}$ , the relation reads

$$\frac{d}{dt} \langle \mathbf{r} \cdot \mathbf{p} \rangle = i \langle [H, \mathbf{r} \cdot \mathbf{p}] \rangle$$

From the definition of the momentum operator, the  $\mathbf{r} \cdot \mathbf{p}$  operator can be written as

$$\mathbf{r} \cdot \mathbf{p} = -ix \frac{\partial}{\partial x} - iy \frac{\partial}{\partial y} - iz \frac{\partial}{\partial z}$$

The Hamiltonian is given by

$$H = T + V = -\frac{1}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + V(r)$$

By observing that all the commutators of derivatives with respect to a different variable is zero, there is only three terms that contributes. By applying the commutation relation for momentum and position, the commutator can be written as

$$i[H, \mathbf{r} \cdot \mathbf{p}] = -\frac{1}{m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) - x \frac{\partial V}{\partial x} - y \frac{\partial V}{\partial y} - z \frac{\partial V}{\partial z} = 2T - \mathbf{r} \cdot \nabla V$$

The time derivative of the operator  $A = \mathbf{r} \cdot \mathbf{p}$  is thus given by

$$\frac{d}{dt} \langle \mathbf{r} \cdot \mathbf{p} \rangle = 2 \langle T \rangle - \langle \mathbf{r} \cdot \nabla V \rangle$$

For stationary states the time derivative is zero, yielding

$$2 \langle T \rangle = \langle \mathbf{r} \cdot \nabla V \rangle$$

The above relation is the virial theorem. For a harmonic oscillator potential  $V = (\omega^2 r^2)/2$ , the right-hand side becomes

$$\mathbf{r} \cdot \nabla V = 2V,$$

thus yielding the virial relation for a harmonic oscillator as

$$\langle T \rangle = \langle V \rangle \tag{2.16}$$

## 3 Method

### 3.1 The VMC Method Using the Metropolis Algorithm

The Metropolis algorithm is implemented with the following prescription [5, p. 463-464]

1. Fix total number of cycles and thermalization cycles. Establish a initial value  $\mathbf{r}$  and define parameters  $\boldsymbol{\alpha} = \{\alpha_1 \dots \alpha_N\}$ . Then calculate  $|\Psi(\mathbf{r}, \boldsymbol{\alpha})|^2$  and define the stepsize when moving from  $\mathbf{r}_i$  to  $\mathbf{r}_{i+1}$
2. Initialize the energy and variance, then start the monte carlo calculation
3. Make a random change in the position of each electron one at a time, i.e calculate  $\mathbf{r}_{i+1} = \mathbf{r}_i + x\delta\mathbf{r}$ , where  $r$  is a random variable  $r \in [0, 1]$  and  $\delta\mathbf{r}$  is a user chosen step length.
4. Then calculate

$$A = \frac{P(\mathbf{r}_{i+1})}{P(\mathbf{r}_i)}$$

If  $A \geq s$  where  $s$  is a random number  $s \in [0, 1]$ , the new position is accepted, else stay at the same place.

5. If the step is accepted, set  $\mathbf{r}_i = \mathbf{r}_{i+1}$
6. Update the energy and variance
7. When the monte carlo sampling is finished, calculate the mean energy and standard deviation
8. Finally collect results by writing to file

#### 3.1.1 Step Length for the Metropolis Random Walker

When employing the Metropolis Algorithm, we want the random walker to efficiently walk through the relevant parts of configuration space and produce a set of states approximating the distribution given by the trial wave function. The challenge becomes choosing the correct step length when proposing a new state. If chosen too large, the new state is likely very remote, resulting in a very low acceptance amplitude and high rejection of the new state. The electrons will therefore often be stuck in the same spots many iterations in a row, resulting in an inefficient sampling of different states. Choosing a small step size will result in the new state have a similar probability as the old, and therefore the acceptance amplitude will be close to unity and most of the states will be accepted. However, the electrons advances very little each iteration due to the small step size. By requiring a roughly 50% acceptance rate, we establish a compromise in acceptance rate and distance moved each iteration, resulting in a maximization of the efficient movement.

Inspired by [8], we employ a scheme that dynamically tweaks the step size during the thermalization cycles to ensure an approximate 50% acceptance rate. The acceptance rate is evaluated several times during the thermalization cycles, by evaluating the ratio of accepted states and number of cycles time number of particles. The step size is then multiplied with twice this ratio. If the ratio is more than 0.5, the step size increases. Likewise, if the ratio

is less than 0.5, the step size decreases. This automatic adjustment ensures that the ratio approaches 0.5.

### 3.1.2 Optimization of Variational Parameters

When estimating the analytical wave function with  $\Psi_{T_1}$ , given by Equation (2.10), the variational parameter  $\alpha$  must be chosen so that the total energy is minimized.

With  $\Psi_{T_2}$ , given by Equation (2.13), both the variational parameters  $\alpha$  and  $\beta$  must be varied. The strategy is to first use the  $\alpha$  found for  $\Psi_{T_1}$  and then vary  $\beta$  in order to find the lowest energy as function  $\beta$ . Thereafter,  $\alpha$  is varied in order to see whether an even lower energy can be found and so forth.

## 3.2 Non-interacting System of Electrons

With the implementation in place, the expectation value of the energy and the energy variance of the non-interacting electrons as functions of the variational parameter  $\alpha$  with  $\Psi_{T_1}$ , given by Equation (2.10), will be plotted. The simulated energy functional will be compared to the corresponding closed form expression given by Equation (2.15).

A three-dimensional plot of one electron's positional distribution as function of the number of Monte Carlo cycles will also be presented.

## 3.3 Interacting System of Electrons without Jastrow Factor

In similar fashion as in the previous section, the expectation value of the energy and the energy variance of the interacting electrons as functions of the variational parameter  $\alpha$  with  $\Psi_{T_1}$  will be plotted.

Next, the stability of the calculations of the energy  $E_{0,\text{VMC}}$  and energy variance  $\sigma^2$  as functions of the number of Monte Carlo cycles will be studied for oscillator frequencies  $\omega = 0.05, 0.25, 1$  and the interacting system with  $\Psi_{T_1}$ . The results will be presented in a table. The energy results will be compared with the exact results,  $E_{0,\text{Exact}}$ , provided by Taut [1], with the discrepancy between them also tabulated. The relative error is, in general, given by

$$\eta = \left| \frac{v - v_{\text{approx}}}{v} \right|, \quad (3.1)$$

where  $v$  is some value and  $v_{\text{approx}}$  the approximation to it. The results  $E_{0,\text{Jacobi}}$  obtained with the Jacobi rotation method by the authors in [2] will also be listed for comparison.

Having found an optimal number of Monte Carlo, the corresponding energy and energy variance for the different oscillator frequencies will be extracted and tabulated in a separate table for later comparisons, along with the mean relative distance between the electrons.

## 3.4 Interacting System of Electrons with Jastrow Factor

Using the optimal number of Monte Carlo cycles, the energy, energy variance, and mean relative distance between the electrons will be computed for the same oscillator frequencies

as previously and the interacting system with  $\Psi_{T_2}$ , given by [Equation \(2.13\)](#). The results will be tabulated.

A table with the relative error between both the energies and relative distances for  $\Psi_{T_1}$  and  $\Psi_{T_2}$  will also be presented.

### 3.5 The Quantum Oscillator Virial Relation

In order to test the virial relation given by [Equation \(2.16\)](#), the expectation values of the kinetic,  $\langle T \rangle$ , and potential,  $\langle V \rangle$ , energy will be computed for different oscillator frequencies. A plot of the ratio  $\langle T \rangle / \langle V \rangle$  will be presented for both the non-interacting and interacting case.

## 4 Results

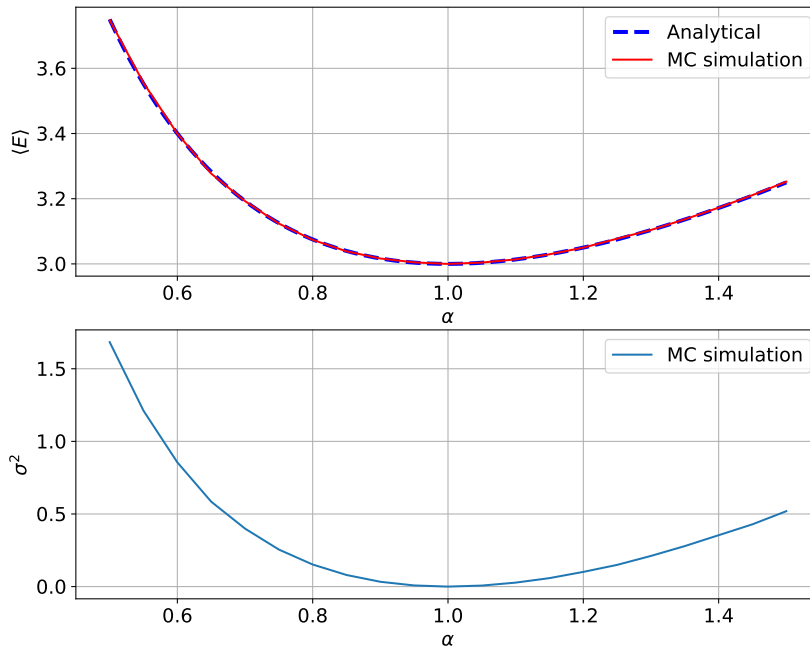
### 4.1 The VMC Method Using the Metropolis Algorithm

The programs containing the implementations of the variational Monte Carlo method using the (brute-force) Metropolis algorithm, as well as accompanying programs that produces all the results presented in this project, can be found at the GitHub repository

<https://github.com/nicolossus/FYS3150/tree/master/Project5>

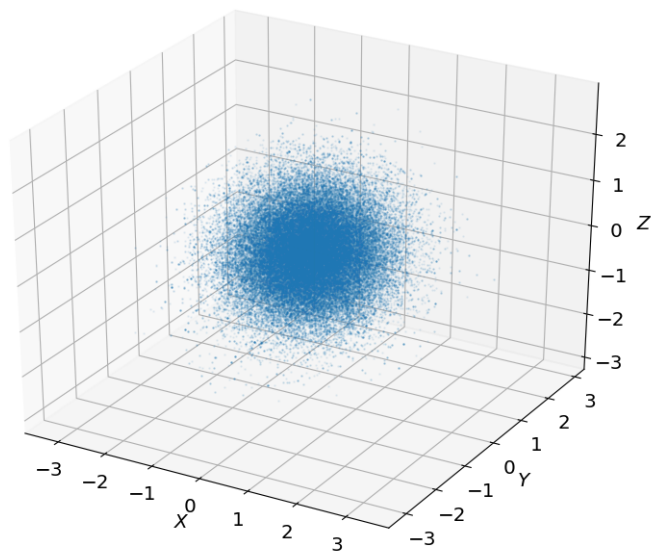
### 4.2 Non-interacting System of Electrons

Figure 4.1 shows a comparison of the analytical and numerical solutions to Equation (2.1) as a function of the variation parameter  $\alpha$ . The plot also present the variance as a function of  $\alpha$ . The plot is generated using the wavefunction Equation (2.10), with a total number of monte carlo cycles  $N = 10^6$ .



**Figure 4.1:** This is a plot of the energy  $\langle E \rangle$  and variance  $\sigma^2$  in the non-interacting case as a function of the parameter  $\alpha$ . The first plot presents a comparison of the analytical and numerical solution, and the second is the variance of the numerical solution. These plots are generated for a total of  $N = 10^6$  monte carlo cycles.

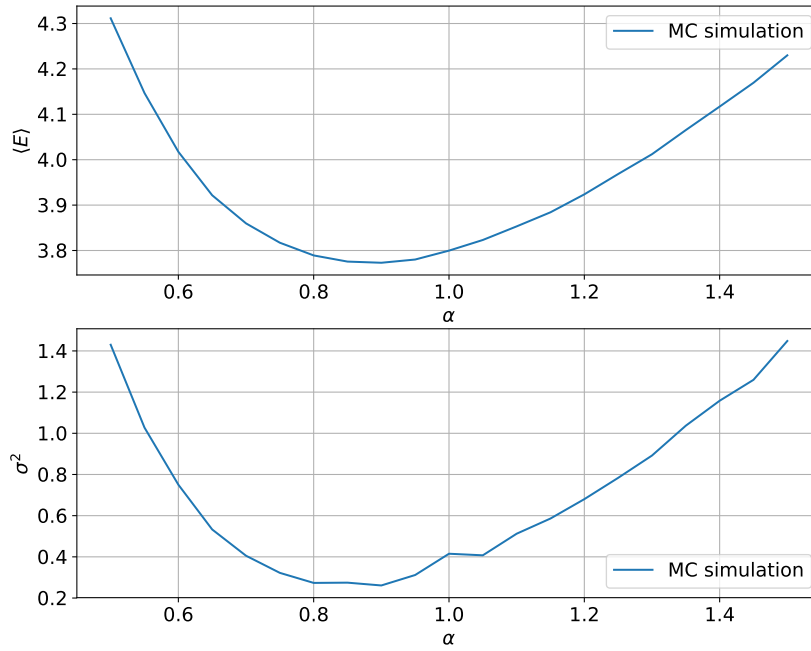
Figure 4.2 shows a visualisation of the position sampling of one electron using the Metropolis algorithm, described in Section 3.1. The plot is generated using  $N = 10^5$  monte carlo cycles.



**Figure 4.2:** *This is a plot of the position of one electron trapped in a harmonic oscillator potential. The plot is generated using  $N = 10^5$  monte carlo cycles.*

### 4.3 Interacting System of Electrons without Jastrow Factor

Figure 4.3 shows a plot of the energy and variance for the interacting case as a function of the parameter  $\alpha$ . The plot is generated using the trial wavefunction [Equation \(2.10\)](#), with a total number  $N = 10^6$  monte carlo cycles.



**Figure 4.3:** This is a plot of the energy  $\langle E \rangle$  and variance  $\sigma^2$  in the interacting case as a function of the parameter  $\alpha$  and with  $N = 10^6$  monte carlo cycles.

Table 4.1 presents the results generated using Metropolis algorithm in order to solve the problem of two interacting electrons in a harmonic oscillator potential, as described in Section 3.1. These results are then compared with the exact result and the result obtained in project 2 [2]. Using trial wavefunction Equation (2.10) and local energy Equation (2.12), we minimize the energy by varying the parameter  $\alpha$ , which yields  $\alpha = 0.879375$ .



**Table 4.1:** Here,  $\omega$  is the oscillator frequency,  $E_{0,\text{exact}}$  the analytical ground state energies retrieved from [1],  $N$  the number of Monte Carlo cycles,  $E_{0,\text{VMC}}$  the ground state energy generated by the variational Monte Carlo method,  $\eta$  the relative error, given by Equation (3.1), between  $E_{0,\text{exact}}$  and  $E_{0,\text{VMC}}$ ,  $\sigma^2$  the variance of  $E_{0,\text{VMC}}$ , and  $E_{0,\text{Jacobi}}$  the ground state energy generated by the Jacobi rotation method in [2].

$\omega$	$E_{0,\text{exact}}$	$N$	$E_{0,\text{VMC}}$	$\eta$	$\sigma^2$	$E_{0,\text{Jacobi}}$
0.05	0.2500	$10^3$	0.3211	0.28	0.0134	0.2499
		$10^4$	0.3157	0.26	0.0127	
		$10^5$	0.3179	0.27	0.0164	
		$10^6$	0.3181	0.27	0.0151	
0.25	1.0000	$10^3$	1.1336	0.13	0.1533	0.9999
		$10^4$	1.1337	0.13	0.0756	
		$10^5$	1.1309	0.13	0.0761	
		$10^6$	1.1302	0.13	0.0682	
1	3.5580	$10^3$	3.7496	0.05	0.1927	3.5289
		$10^4$	3.7719	0.06	0.2119	
		$10^5$	3.7725	0.06	0.2479	
		$10^6$	3.7743	0.06	0.2660	

Table 4.2 shows the energy  $\langle E \rangle$  variance  $\sigma^2$  for a few selected values extracted from Table 4.1 along with the mean separation between the electrons  $\langle r_{12} \rangle$ . The plot is generated using  $\omega = 0.05$ ,  $\omega = 0.25$  and  $\omega = 1$ , with a total number of monte carlo cycles  $N = 10^6$ .

**Table 4.2:** Here,  $\omega$  is the oscillator frequency,  $E[\psi_{T1}]$  is the ground state energy by VMC,  $\sigma^2[\psi_{T1}]$  is the variance and  $\langle r_{12} \rangle$  is the mean separation between the electrons.

$\omega$	$E[\psi_{T1}]$	$\sigma^2[\psi_{T1}]$	$\langle r_{12} \rangle$
0.05	0.3181	0.0151	7.60372
0.25	1.1302	0.0682	3.40358
1	3.7743	0.2660	1.70174

## 4.4 Interacting System of Electrons with Jastrow Factor

Table 4.2 shows the energy  $\langle E \rangle$ , variance  $\sigma^2$  and mean separation between the electrons  $\langle r_{12} \rangle$ , for  $\omega = 0.05$ ,  $\omega = 0.25$  and  $\omega = 1$ . The results is generated using the trial wavefunction Equation (2.13) and local energy Equation (2.14). We minimize the energy by varying the parameters  $\alpha$  and  $\beta$ . This yields  $\alpha = 0.992344$ ,  $\beta = 0.284687$ . This is generated using a total number of monte carlo cycles  $N = 10^6$ .

**Table 4.3:** Here,  $\omega$  is the oscillator frequency,  $E[\psi_{T2}]$  is the ground state energy by VMC,  $\sigma^2[\psi_{T2}]$  is the variance and  $\langle r_{12} \rangle$  is the mean separation between the electrons.

$\omega$	$E[\psi_{T2}]$	$\sigma^2[\psi_{T2}]$	$\langle r_{12} \rangle$
0.05	0.3003	0.002737	8.1439
0.25	1.0960	0.003727	3.6888
1	3.7302	0.0002341	1.8146

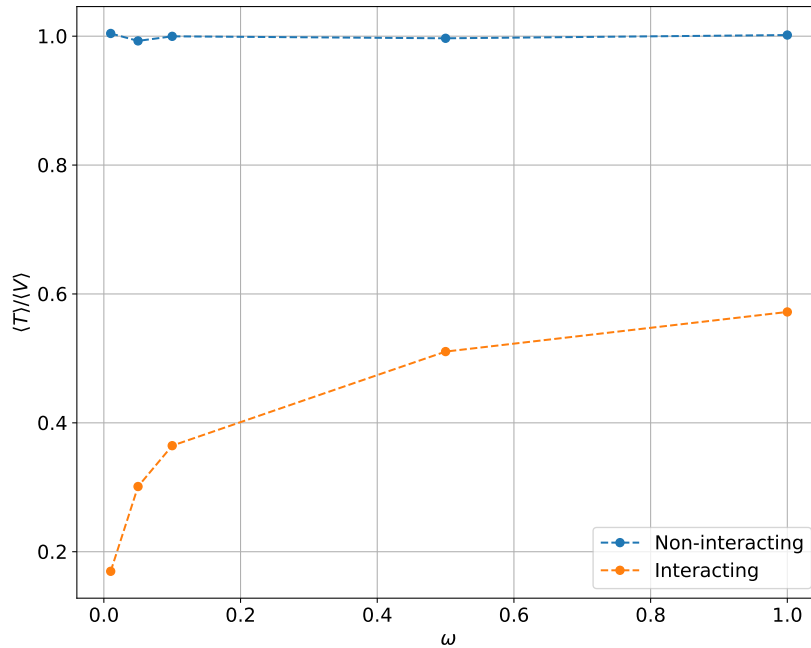
Table 4.4 shows the result of calculating the difference between the energies using Equation (2.10) and Equation (2.13), for  $\omega = 0.05$ ,  $\omega = 0.25$  and  $\omega = 1$ . The table also presents the relative error  $\eta$ , given by Equation (3.1)

**Table 4.4:** Here,  $\omega$  is the oscillator frequency,  $\eta_E$  is the relative decrease in energy between with and without the Jastrow factor, and  $\eta_R$  is the relative increase in mean separation  $\langle R_{12} \rangle$ .

$\omega$	$\eta_E$	$\eta_R$
0.05	0.056	0.071
0.25	0.030	0.084
1	0.012	0.066

## 4.5 The Quantum Oscillator Virial Relation

Figure 4.4 is a plot of the virial relation for a harmonic oscillator, given by Equation (2.16). The plot presents the relation as a function of oscillator frequency  $\omega$ , using non-interacting Hamiltonian with wavefunction given by Equation (2.10), and the interacting Hamiltonian using the wavefunction Equation (2.13). The plot is generated using  $N = 10^6$  monte carlo cycles.



**Figure 4.4:** This is a plot of the ratio between the kinetic and potential energy as a function of oscillator frequency. The plot is generated using  $N = 10^6$  monte carlo cycles.

## 5 Discussion

### 5.1 The VMC Method Using the Metropolis Algorithm

When implementing the VMC method with the Metropolis algorithm, the code (see [GitHub](#)) was written with object oriented code. The `VMC` class contains the implementation of the VMC method with the Metropolis algorithm.

The sought acceptance rate of roughly 0.5 was achieved, as verified by a unit test in `test.cpp`. This implementation is, however, a somewhat brute-force approach. The Metropolis algorithm in the `VMC` class could have been extended to include a acceptance rate using a likelihood function to guide the jumps of the Metropolis random walker, i.e. the Metropolis-Hastings algorithm.

In estimating the analytical wave function of the interacting system,  $\alpha$  and  $\beta$  was varied in order to minimize the estimated energy. This was done by the class method `optimize`. This method is called with a value `range`, indicating how wide the algorithm must search for a optimal value, and a value `step`, deciding how many discrete points the search are should be divided in. As initial values,  $\alpha$  was set to be equal to the value that yielded the minimum energy for the trial wave function without the Jastrow factor, and  $\beta$  was set to 0.8. First,  $\beta$  was varied according to `range` and `step`, and the value yielding the smallest energy was kept. Then,  $\alpha$  was varied in the same manner. After tweaking both parameters, `range` was halved to increase the fineness of the tweaking, and the process was started over. This was repeated a total of 10 times.

Even though the `optimize` method of the VMC class produces sensible results, the method as implemented is not fully robust. Since we periodically halve `range` to narrow the search area, it is not unthinkable that we accidentally leave the true minimum outside at some point. Alternatively, one could implement a gradient decent method derived from the local energy to tweak the parameters.

### 5.2 Non-interacting System of Electrons

From [Figure 4.1](#) we see that  $\alpha = 1$  yields the correct expectation value  $\langle E \rangle = 3$  for the non-interacting case. This makes sense, as our choice of trial wave function, given by [Equation \(2.10\)](#), reduces to the analytically correct wave function for this particular value. Since this wave function is an eigenfunction of the Hamiltonian, the local energy reduces to a number rather than a distribution dependent on the  $\mathbf{r}$ , as can be seen by setting  $\alpha = 1$  in [Equation \(2.11\)](#). Being a single number, it follows from [Equation \(2.8\)](#) that the variance in the local energy goes to zero, suggested by [Figure 4.1](#), indicating that we have hit a analytically correct wave function.

As the local energy becomes independent of  $\mathbf{r}$ , just evaluating for  $\alpha = 1$  gives little insight in whether the Metropolis Algorithm is doing something sensible or not. However, [Figure 4.1](#) suggest that the analytical energy [Equation \(2.15\)](#) and the numerical are approximately equal for  $\alpha \in [0.5, 1.5]$ , giving confidence that [Equation \(2.4\)](#) and [Equation \(2.10\)](#) are correctly implemented in the program and that the Metropolis algorithm is working.

[Figure 4.2](#) is a nice visualization of the sample of positions made by the Metropolis Algorithm. The density appears to be larger in the center, which makes sense as the wave function

amplitude is larger in this area. Also some few, more remote points have been sampled. Even though these states have a low probability of occurring, we expect them to do now and then. This suggest that our model preserves ergodicity, meaning that system is able to assume any state with a non-zero probability.

### 5.3 Interacting System of Electrons without Jastrow Factor

For the interacting case using trial wave function, Equation (2.10), Figure 4.3 shows much the same trend as Figure 4.1, all though the variance never reaches zero. This indicates that we at no points manage to hit the analytical wave function, as is to be expected, since the trial wave function is fairly naive and doesn't even satisfy the cusp-condition.

From Table 4.1, we see that the precision is not good, averaging 6% relative error for  $\omega = 1$ , easily outclassed by the energy obtained as the solution of a eigenvalue problem. For lower  $\omega$ , the precision was even worse.

For increasing number of cycles, the relative error did not necessarily decrease, but rather increased in some cases. This can be explained by the fact that we are not technically estimating the analytically energy directly, but rather the energy that our specifically chosen trial wave function yields(the upper bound estimate). However many cycles we use, we can never hope to get an energy closer than that our trial wave function allows. As the relative error is somewhat high, it appears our choice was poor.

Table 4.2 shows that smallet  $\omega$  yields a larger mean distance  $\langle R_{12} \rangle$ . This is expected, as a weaker harmonic potential confines the electrons less strongly, letting the Coulomb interaction push them further apart.

### 5.4 Interacting System of Electrons with Jastrow Factor

Introducing the Jastrow factor, Table 4.4 shows a decrease of roughly 2% in energy and a 7% increase for mean separation for  $\omega = 1$ . For smaller  $\omega$ , the variation was somewhat bigger, indicating that the Jastrow-factor is of some importance in estimating the energy and mean separation of the system.

Since the energies estimated with the Jastrow factor are smaller, the new estimates more strictly binds the actual energy from above, and is hence better. However, from Table 4.3, we see that the new upper bound estimate is 3.7302 a.u., as opposed to the analytical 3.588 a.u. All though marginally better, the estimated upper bound is still some percent larger than the analytical value, and the variance not zero. Even with the Jastrow factor, we struggle to get a trial wave function that manages to yield a precision anything close to that of the Jacobi rotation method.

### 5.5 The Quantum Oscillator Virial Relation

From Figure 4.4, we see that the non-interaction case follows the virial theorem, as the ratio of kinetic to potential energy is approximately 1 independent of  $\omega$ . This is in accordance with Equation (2.16). For the interaction case, the ratio is smaller than 1 and increasing as  $\omega$  increases. This can be explained by the introduced Coulomb term, which adds to

the potential energy of the system and thus decreases the ratio. From the local energy [Equation \(2.14\)](#), we see that both the kinetic energy and harmonic potential scales with  $\omega^2$ . The Coulomb-term does not have the same dependency, and likewise the ratio varies across different  $\omega$ . The system does not follow the virial theorem in the interacting case.

## 6 Conclusion

In this project, the variational Monte Carlo (VMC) method was used with the Metropolis algorithm to evaluate the ground state energy  $E_0$ , the mean relative distance between two electrons  $r_{12}$ , and the expectation values of the kinetic,  $T$ , and potential,  $V$ , energies of three-dimensional two-electron quantum dots (harmonic oscillator-like potentials), both with and without inter-electronic Coulomb interaction. Two trial wave functions  $\Psi_{T_1}$  ([Equation \(2.10\)](#)) and  $\Psi_{T_2}$  ([Equation \(2.13\)](#)), with the latter accounting for the electron-electron interaction and the former not, were constructed with optimal variational parameters found upon minimizing the total energy of the systems.

The simulated energy functional as a function of the variational parameter  $\alpha$  for the non-interacting system with  $\Psi_{T_1}$ , aligned very well with the corresponding closed-form expression given by [Equation \(2.15\)](#).

For the interacting system with  $\Psi_{T_2}$  and oscillator frequency  $\omega = 1$ , the upper bound estimate of the ground state energy was simulated, with  $N = 10^6$  Monte Carlo cycles, to be 3.730 a.u. (atomic units). Compared to the corresponding analytical value 3.558 a.u., it seems like the method struggles to yield a precise estimate of the energy in the interacting case. The choice of variational Monte Carlo seems as a misinformed one, as the method is much more suited for studying system of a large degree of freedom, such as a many-particle system. For a two-electron system, it has been shown in [\[2\]](#) that numerical methods such as matrix diagonalization is much more effective and yields more precise results.

It was also found that the mean relative distance between the two electrons at the energy minimum decreased as the characteristic oscillator frequency of the potential increased.

The virial theorem applied to a quantum harmonic oscillator,  $\langle T \rangle = \langle V \rangle$ , was tested for both the non-interacting and interacting system as a function of  $\omega$ . The former system corresponded well with the virial theorem, whereas the latter did not conform with the theorem. This is, however, expected since the aforementioned virial relation is derived for a non-interacting harmonic oscillator.

## 7 Future Work

The Metropolis algorithm in the **VMC** class can be extended to include a acceptance rate using a likelihood function to guide the jumps of the Metropolis random walker, i.e. the Metropolis-Hastings algorithm.

Even though the estimated energy was not as good as one could hope, the minimum energy wave function obtained by the varying  $\alpha$  and  $\beta$  is still an excellent start for a continuation using diffusive Monte Carlo (DMC), preferably for multiple electrons. Diffusive Monte

Carlo can theoretical come arbitrary close to the exact value, but relies on a fairly good approximation to the wave function to ensure that the result converges.

Even though the `optimize` method of the VMC class produces sensible results, the method as implemented is not fully robust. Since we periodically halve `range` to narrow the search area, it is not unthinkable that we accidentally leave the true minimum outside at some point. Alternatively, one could implement a gradient decent method derived from the local energy to tweak the parameters.

Also, since it is very simple for Monte Carlo methods, the code should be parallelized using e.g. MPI.

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